December 29, 1964

Dr. S. H. Eisman SMUFA - 1312
Frankford Arsenal
Philadelphia, Pennsylvania 19137

Dear Dr. Eisman:

Thank you for your letter of December 17. I am especially grateful to have the references. The very antiquity of much of the work in this field makes it hard to trace. The "computer people" is also mainly me and I will eagerly look for Tabory.

I am sorry about the obscurities in my brief note and hope the more detailed report (almost ready, and I will send you an early copy) will clear some of them up. A path maps onto an edge, so one polygon of course encompasses a genus of rings; one must also give the detailed mapping, which I have done roughly, as you indicate. (See also the morphinan example in the note.) To use your examples, the codes for RRI 6128 and 6310 can be contracted:

6128 (8L(3N)4,,N,,,O.N,C,,,4)

6310 (8L-4,,,N,,3,,,C,4) or in a more compact form,

(8L7-c,N,3,C,4)

These may be clarified by the attached work sheet; also the idea of the ortho-mesh from a couple of pages of the draft report.

I generally agree about manipulating polygons, and especially on the computer. The polyhedral viewpoint was very useful in understanding the isomorphisms and the symmetries, the orthomeshes, and the rules about non-polygonal graphs like 8M. Of course, the fundamental algebra is the incidence matrix, but we also have to visualize its allowable permutations.

I have nothing against non-planar graphs, but didn't feel obliged to spin many hypothetical examples before any had been made. Canonical forms fall out quite straightforwardly as soon as there is any occasion for them. Conformational varieties can be grafted onto the system too, e.g., also hindered rotations, etc. I wouldn't want to put them into a generator algorithm until I could predict their resolvability more smoothly.

As to "polycenes", I am not so enthusiastic about them except for fairly straight-forward hexacyclics, which still leaves a substantial market. It is not hard to find a representation for other varieties, but the rules get very fussy for canonical forms, so the advantage disappears. In realistic terms, should we spend much time on the fascinating curiosities of dozens of rings?

S.H. Eisman

You may have gotten a bad copy of the figure and I enclose another. (Don't memorize those labels. I have already felt constrained to put them in a more sensible order!)

Anyhow, it looks as if the field is just beginning to get the mathematical analysis it deserves. What a rheumy time for CA and IUPAC to standardize!

Sincerely yours,

Joshua Lederberg
Professor of Genetics